METHODS AND SYSTEMS FOR PREPARING VIRTUAL REPRESENTATIONS OF MOLECULES

ABSTRACT OF THE DISCLOSURE

[0098] Methods and systems for improving virtual representations of large molecules provide a "prepared" virtual representation of the target protein. The prepared virtual representation of the target protein is useful for further *in-silico*, or computer processing. Further processing can include, without limitation, designing of small molecules that will potentially bind and/or interact with the target protein. In accordance with the invention, one or more features of the virtual representation of the protein are assessed. One or more of a variety of assessments can be performed including, without limitation, analyzing for completeness (e.g., missing and/or incomplete residues and/or side chains), identifying missing (typically smaller) atoms, determining ionization states (i.e., protonated or not), determining orientation of bonds, and/or identifying atoms that are not part of the protein. The virtual representation of the protein is then modified, as needed, based, at least in part, on the assessment(s). Modification can include, without limitation, refining, improving, tailoring, editing, and/or revising the virtual representation of the protein.